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IHPRPT Phase III
Solid Rocket Motor Modeling Program

Status of Advanced Two-Phase Flow Model Development for SRM Chamber Flow Field and Combustion Modeling

(109-A0031)

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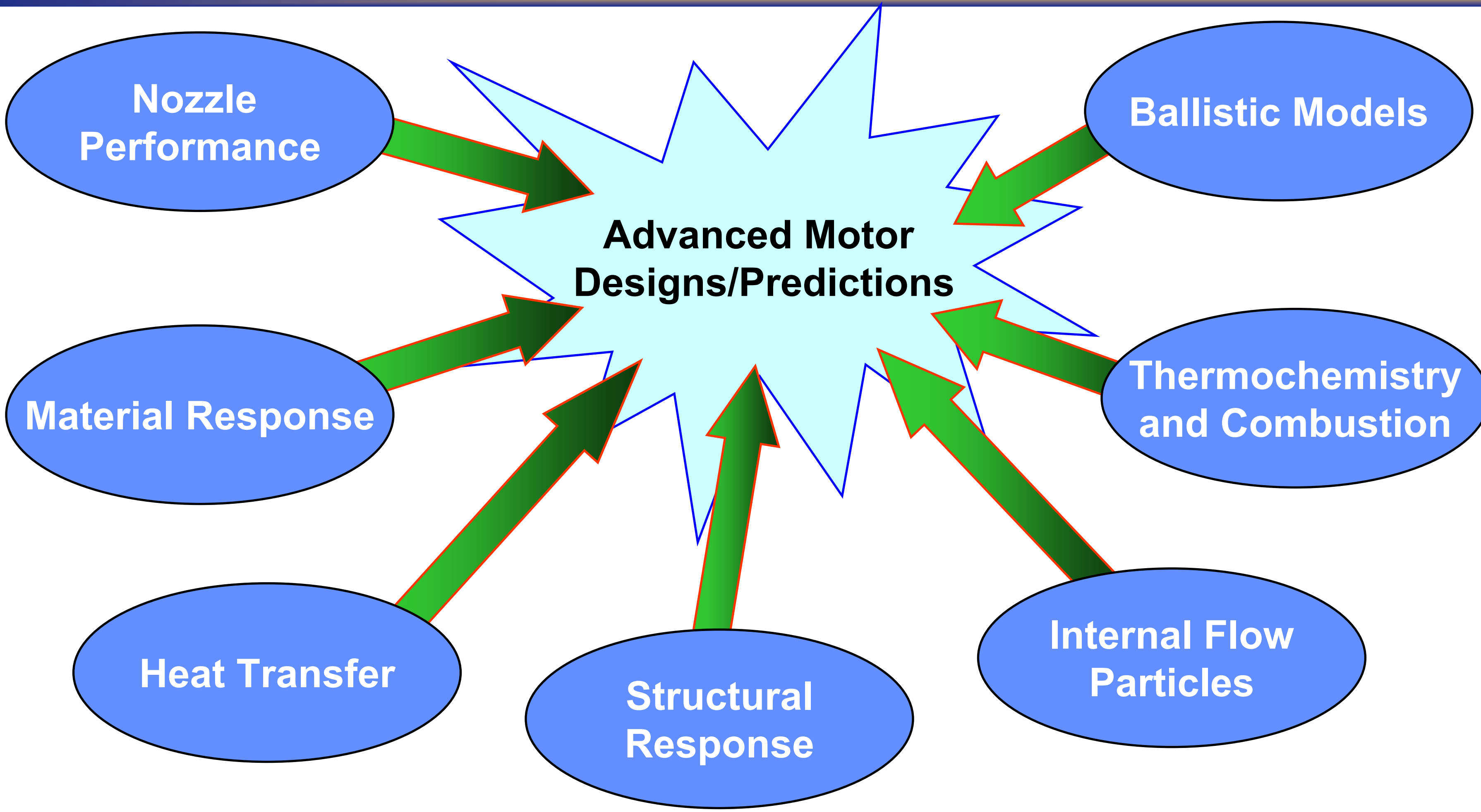
Outline

- Overview of Aerojet's IHPRPT Modeling and Simulation (M&S) Program for Solid Rocket Motors (SRM)
- Aerojet Team Members and Organizational Interfaces
- Model Complexity and Aerojet Approach
- Brief Description of Two-Phase Flow Model with Combustion
- CFD Computing Environment (Runtime Choices)
- Keys to Success
- Model Verification and Validation
- MNASA SRM Test Data
- Concluding Remarks

Goals and Objectives of SRM M&S Program



Physics-Based Models Reduce Development Risks for Next Generation Technology Motors

Role of Modeling and Simulation Task

Major Tasks
- Particle Sizing/Dynamics Models
- Al Combustion and Distributed Chemistry Models
- Boundary Layer Module
- Fluid Mechanics Model Improvements
- Interface Development

Ballistic Burnback → Combustion Thermochemistry

Combustion Thermochemistry → Complex Geometry (3-D Flowfield)

Combustion Thermochemistry → Particle Models

Complex Geometry (3-D Flowfield) → Two-Phase Flow Coupled

Particle Models → Two-Phase Flow Coupled

Two-Phase Flow Coupled → Nozzle Performance Loss Mechanisms Boundary Layer, Divergence, Two-Phase

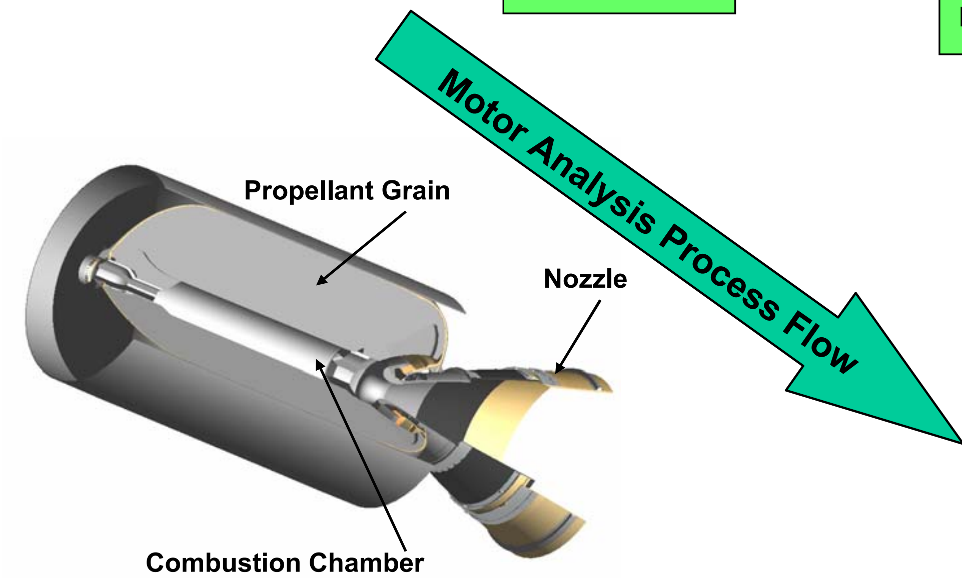
Two-Phase Flow Coupled → Heat Transfer Models Coupled With Gas

Heat Transfer Models Coupled With Gas → Nozzle Performance Loss Mechanisms Boundary Layer, Divergence, Two-Phase

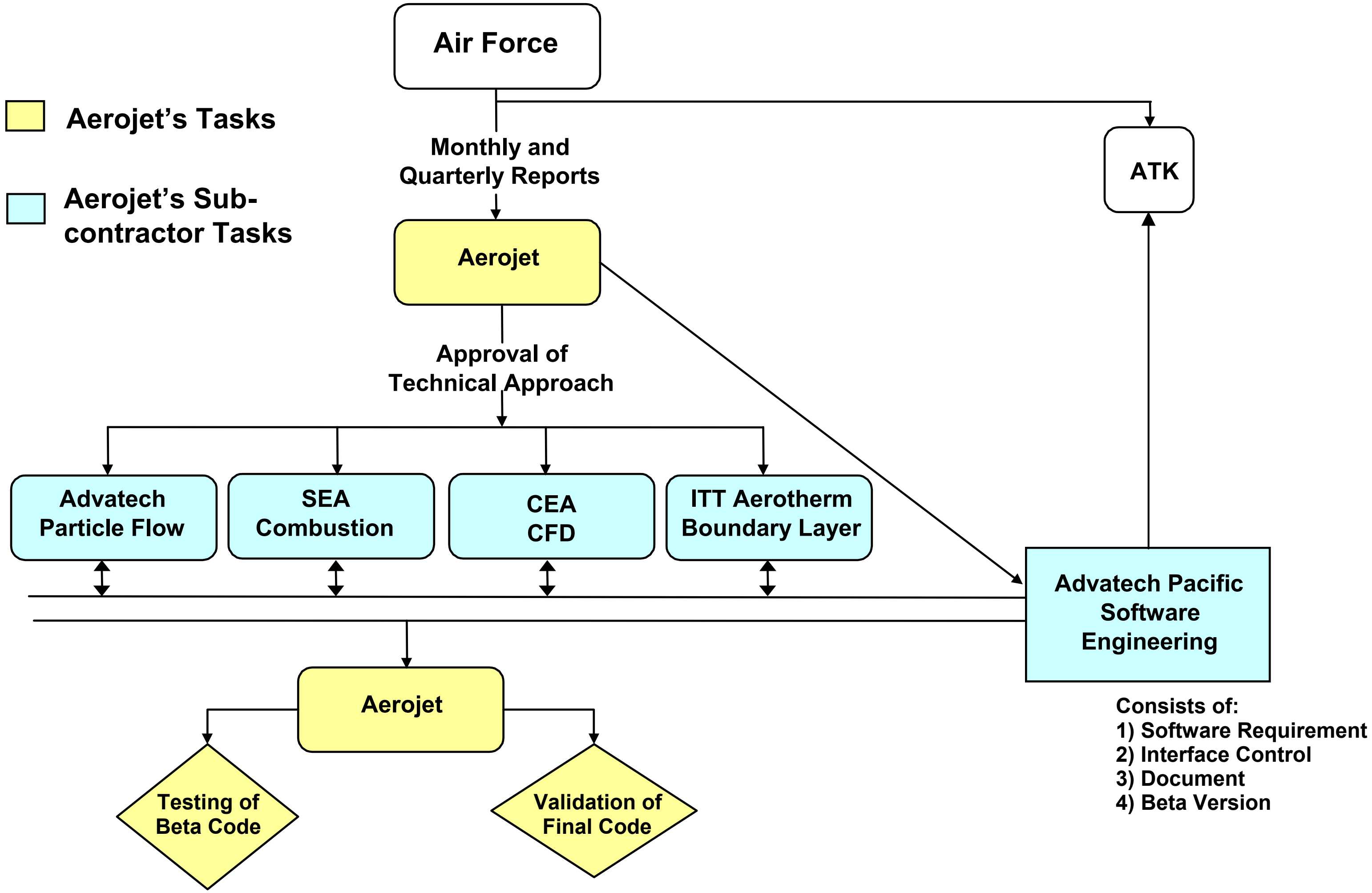
Heat Transfer Models Coupled With Gas → Material Response Thermal, Ablation

Material Response Thermal, Ablation → Nozzle Performance Loss Mechanisms Boundary Layer, Divergence, Two-Phase

Material Response Thermal, Ablation → Structural Response



IHPRPT M&S Program Organizational Interfaces



Model Complexity Approach

- Allow variable complexity level of analysis to be brought to bear at user discretion
  - Simplified models for preliminary design and motor/component sizing
  - Engineering models for detailed design and validation, performance estimates
  - Research models for investigating new design approaches, advanced materials, failure or anomaly investigation, etc.
- Final product targeted at engineering model level of complexity
  - Utilize models for motor detailed design phase (PDR/CDR)
  - Assume 2-3 month design cycle, CDR level of analysis capability
  - Allow component design validation via analysis
- Flexibility will be built into model to allow user to access more sophisticated research models when appropriate

The Aerojet Approach

- **Provide an analysis/design architecture and capability that:**
  - can optionally range from simple/fast/approximate to highly complex/accurate.
  - appropriately treats conventional as well as unconventional configurations.
  - may readily be used by junior/moderately skilled as well as senior/highly skilled analysts.
  - is both practical in configuration assessment as well as serves as a research tool for advanced concepts/environments.
  - may readily grow and change as new features and methodologies become available in the future.
  - has a high level of GUI features to facilitate its use by any skill level analyst.

The above goals are not necessarily conflicting if the architecture has been planned and executed properly. The Aerojet plan does just that.

The Aerojet Approach (Continued)

- The core of the approach is an accurate, flexible, and powerful CFD code (MaxS) which permits the user to select the level of physics sophistication while simultaneously selecting the discretization level appropriate to the user's current task needs.
- To the CFD core we are adding advanced physics models for complex chemistry, particulate treatments, and sophisticated boundary layer analyses.
- The GUI has been expanded such that various physics models and features can be easily selected. Pertinent data for various gases, particulates, and other material properties are archived to reduce the required input for a given problem to minimal levels.
- The pre-existing flexible geometric capability has been expanded to permit the consideration of moving boundaries such as regression, erosion, gimbal motion, as well as structural deformations.

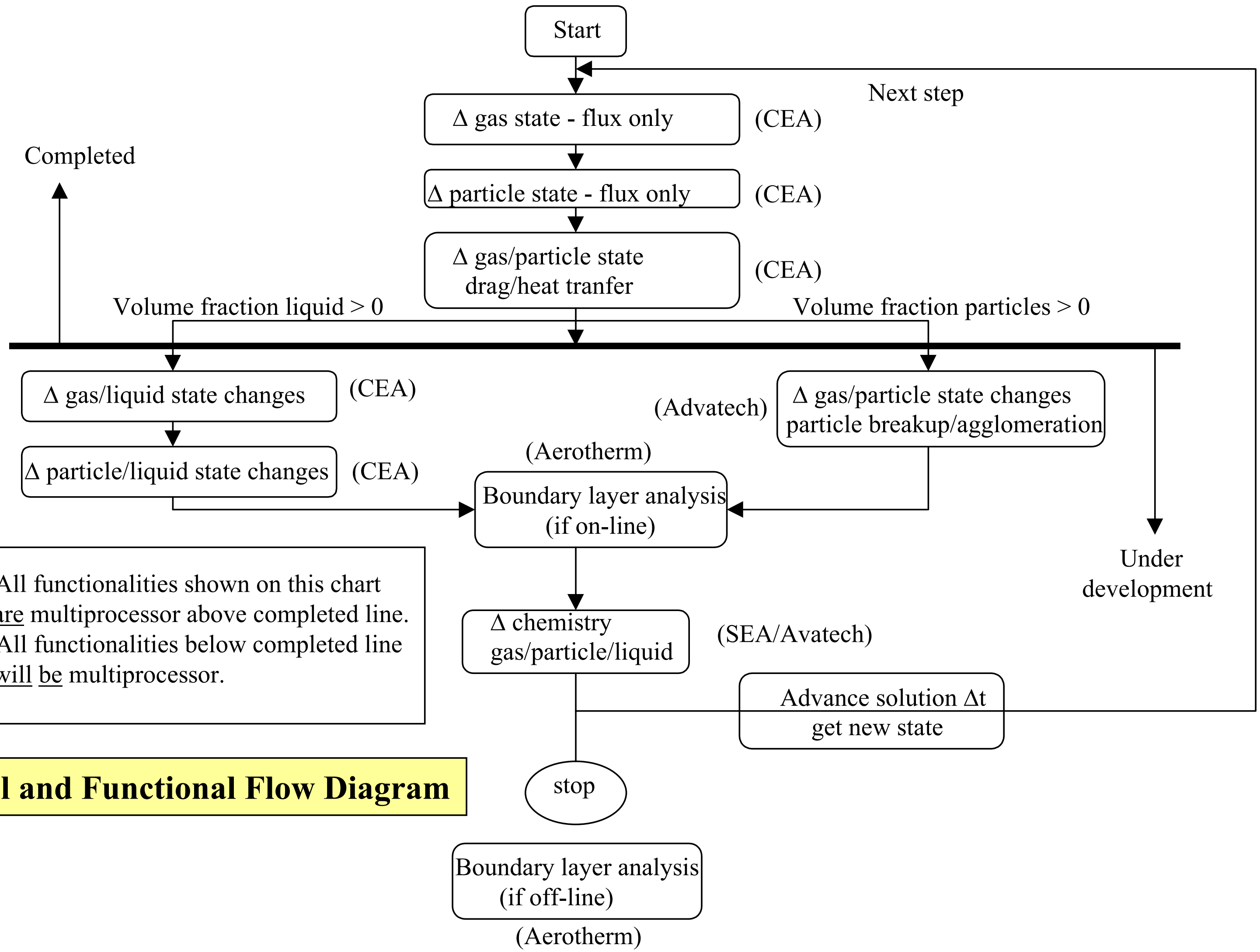
Model Flexibility

- Gas properties description: tabular/equilibrium/finite rate
- Grid definition: MaxS/PATRAN/FLUENT/STEP (any source)
- Boundary layer: CFD to the wall or specialized analyses which optionally may be employed within the core analysis or as post processing features.
- Particulate effects: various models are selectable to govern particle behavior.
- Motion: rigid body or deforming surfaces utilize MaxS or other sources for moving/deforming grid definition.

Proposed Features for 2-Phase Flow Models

- **Physical Processes to Consider:**
  - Al particle melting and agglomeration at propellant surface
  - Al particle combustion and droplet size change in chamber
  - Al and Al_2O_3 particle trajectories and interactions with gas flowfield
  - Al and Al_2O_3 particle coalescence and breakup in chamber and nozzle flowfields
  - Shattered Al particle combustion in nozzle
  - Al_2O_3 accumulation (i.e. slag pooling) and flow across insulation and nozzle surfaces
  - Impacts on boundary layer heat transfer to ablatives due to two-phase flow
  - Thermochemical ablation mechanisms in the presence of two-phase flow
  - Particle impact phenomenon - both subsonic and supersonic conditions

Appropriate Interfaces Identified for Two Phase Flow Simulation



Note: o - All functionalities shown on this chart are multiprocessor above completed line.
o - All functionalities below completed line will be multiprocessor.

Technical and Functional Flow Diagram

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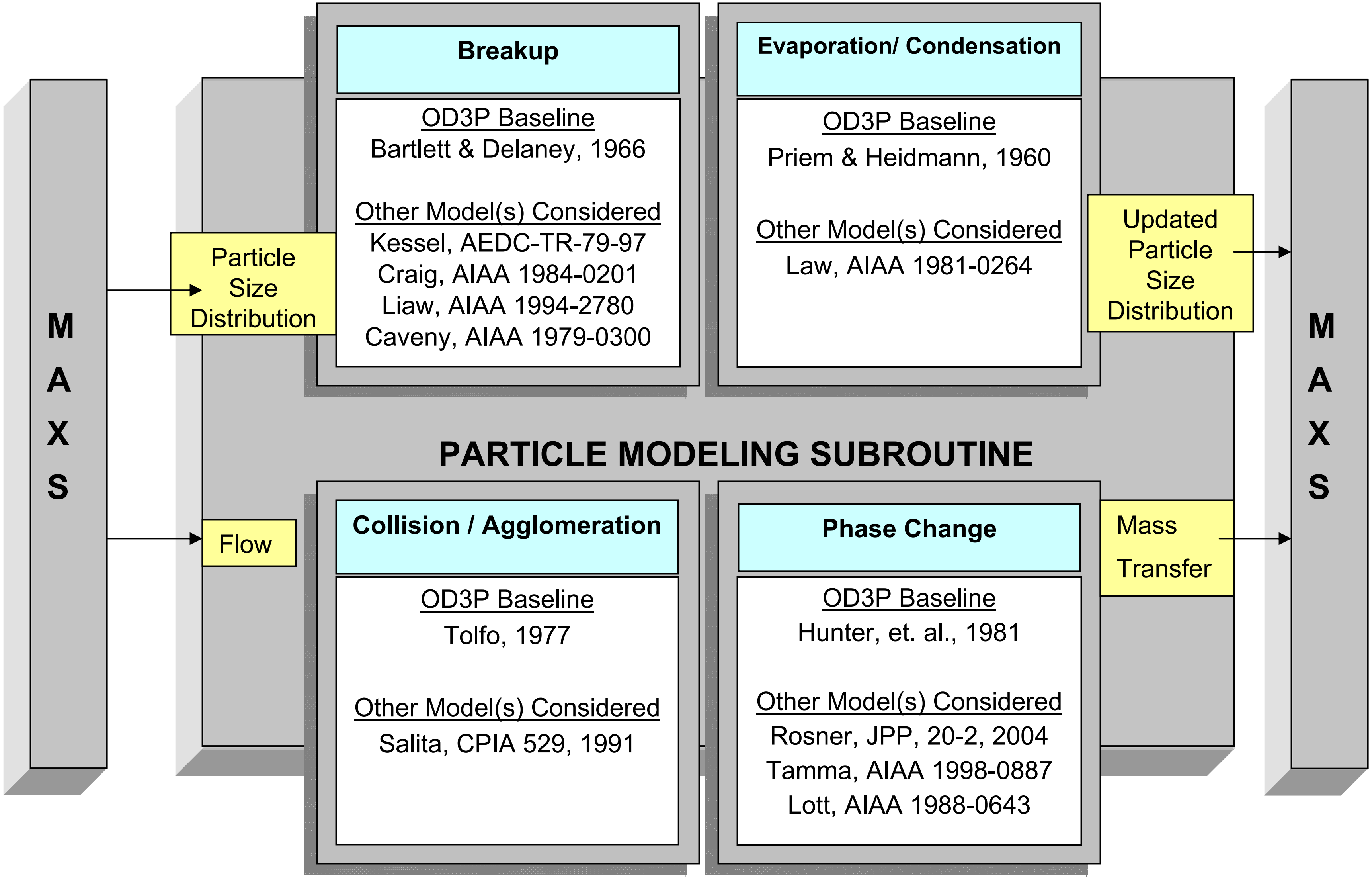
Particle Modeling Approach

- OD3P Modeling approach is our baseline
  - 1980 SOTA, well documented
  - Easily implemented in CFD Codes
- OD3P Particle model considers all reasonably accepted phenomena using individual modules
  - Particle phase change module (solidification/crystallization/melting)
  - Particle mass transfer between phases module (evaporation/condensation)
  - Particle break-up module
  - Particle coagulation module
- Once OD3P baseline is implemented, all other candidate models obtained from literature searches will be evaluated as UPGRADES TO BASELINE

Layout of Particle Subroutine



Aluminum Combustion and Particle Size Distribution

- The key to both aluminum combustion and particle size distribution is being able to model the size of the aluminum agglomerate coming off the surface of the propellant.

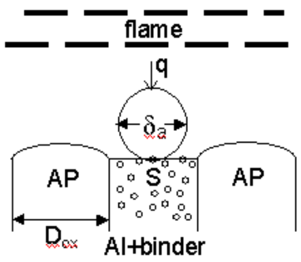
- Current engineering state of the art for agglomeration models are the “analytic” pocket models of Kovalev or Cohen, or empirical fits to measured data such as Hermsen’s correlation in SPP.

- The detailed models of Beckstead, Babuk, UIUC CSAR, and others are not suitable for 3-D CFD solutions due to excessive computational requirements.

- Models of the D^2 type for burning Aluminum are required. Beckstead’s and Hermsen’s models are likely candidates. Both models require the initial Al particle size and the local concentration of oxidizing species.

Data Requirements for Agglomeration Models

Question: Where does the required data come from?



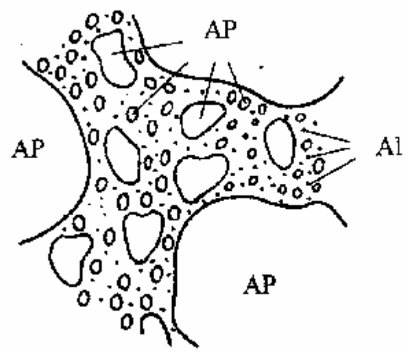
Kovalev's Model

Controlling Parameters

Oxidation of aluminum rate equation

$$\frac{d\eta_a}{dt} = \frac{K_a}{\eta_a}\exp(-E_a / R_0 T_a)$$

E_a determines ignition temperature



Premixed Gas Flame Temperature Equation

$$CpM_T\, dT_g \big/ dz - \lambda\, d^2 T_g \big/ dz^2 = Q_g \psi(Y_1, Y_2, T_g)$$

Q_g and controlling amount of oxidizer, Y_1, or fuel, Y_2, determine the resultant premixed flame temperature

Kovalev, O. B., "Motor and Plume Particle Size Prediction in Solid-Propellant Rocket Motors," *Journal of Propulsion and Power*, vol. 18, no. 6, Nov.-Dec. 2002, pp. 1199-1210

Simple One Step Burning Models for Al

Beckstead's (2000) Model[1]:

$$\frac{d(m_{Al})}{dt} = -\frac{\pi}{2}\rho_{Al}\frac{k}{1.8}D_p^{1.2}$$

$$k = f(X_{eff}, P_c^{0.1}, T^{0.2})$$

$$X_{eff} = 0.22[CO2] + 0.6[H2O] + [O2]$$

Hermsen's Model[2]:

$$\frac{d(m_{Al})}{dt} = -\frac{\pi}{2}\rho_{Al}\frac{k}{1.8}D_p^{1.2}$$

$$k = 8.3314x10^{-5} A_k^{0.9} P_c^{0.27} Sh/2$$

$$A_k = 100([CO2] + [H2O] + [O2] + [OH] + [O])$$

[1] Beckstead, M.W., Newbold, B.R. and Waroquet, C. "A Summary of Aluminum Combustion," *37th JANNAF Combustion Meeting,* CPIA No. 701, Vol. 1, Nov. 2000, pp. 485-504

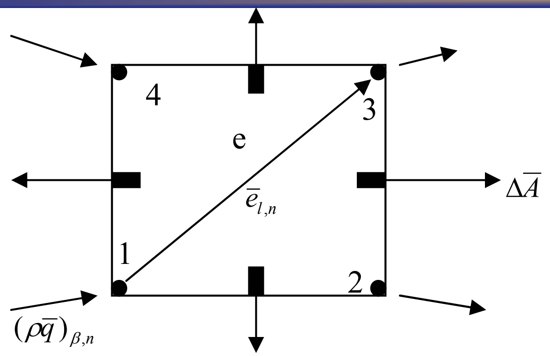
[2] Hermsen, R.W., "Aluminum Combustion Efficiency in Solid Rocket Motors," AIAA Paper 81-0038, 1981.

Distributed Combustion

- **Thermochemistry**
  - Gas phase transport properties as well as the concentrations of oxidizing species are required to track burning droplets.
  - For computational efficiency, tables of equilibrium properties need to be prepared. The independent variables for the table look-up are the amount of unburned Al, amount of Al_2O_3, elemental composition of the gas phase, and two independent thermodynamic properties, e. g., P and T. Initially, the table look-up model will consider gas phase composition to depend only on amount of unburned Al.

- **Droplet Burning Model**
  - For CFD solutions, the local droplet size distribution including the amounts of Al and Al_2O_3 and the concentrations of oxidizing species are required. The droplet burning models will supply the amount of Al converted to Al_2O_3 and droplet size change. The equilibrium thermodynamic properties look-up routine will determine the resultant gas properties and heat release.

Particle Phase Treatment



Typical element - N corners - n=1,N

- $(\dot{\rho}_\beta V)_e = -\int_{cs}(\rho\bar{q})_\beta \bullet d\bar{A} \;\; = -\sum_{n=1}^{N}[(\rho\bar{q})_\beta \bullet \Delta\bar{A}]_n \;\;, \quad \beta = 1, B$
- Corner flux piece: $(\dot{\rho}V)_{\beta,n} = -[(\rho\bar{q})_\beta \bullet \Delta\bar{A}]_n$

  Let amount of corner flux at (n) distributed to node (l) be $\xi_{l,n}$
- Conservation requires that: $\sum_{l=1}^{N}\xi_{l,n} = 1$

<u>The conservation equations provide no information regarding an appropriate distribution.</u>

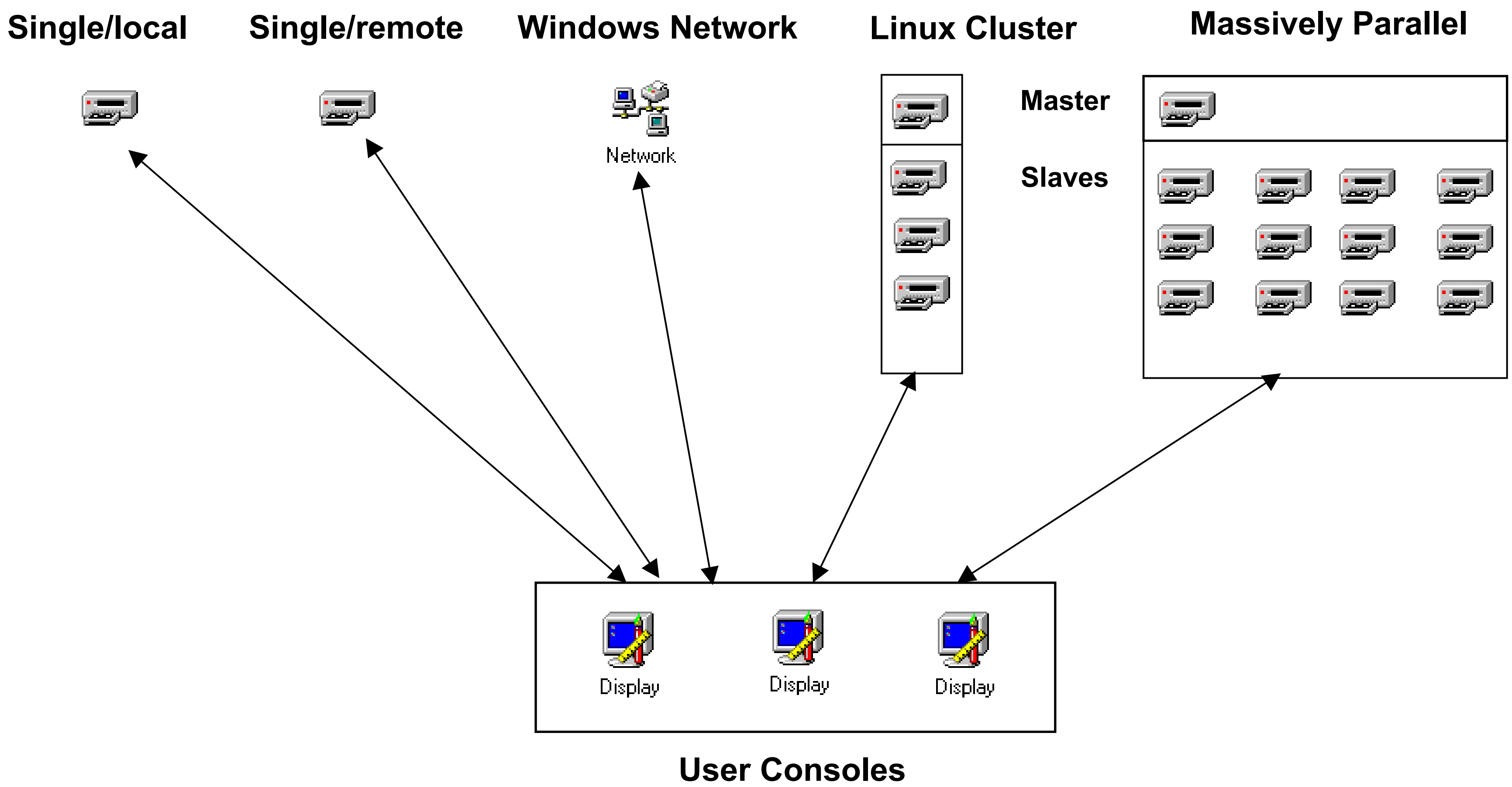
If there is no gas present, it is obvious that a Lagrangian point of departure would allow <u>no</u> backward communication. The following distribution approach satisfies that observation.

- Incoming $[(\rho\bar{q})_\beta \bullet \Delta\bar{A}]_n \le 0$ $\quad \left\{\begin{matrix} \xi'_{l,n} = 0 \;\;, \;\; [(\rho\bar{q})_\beta \bullet \bar{e}_l]_n \le 0 \\ \xi'_{l,n} = [(\rho\bar{q})_\beta \bullet \bar{e}_l]_n \;\;, \;\; [(\rho\bar{q})_\beta \bullet \bar{e}_l]_n \ge 0 \end{matrix}\right\}$ $\quad$ for $\quad l \ne n$
- Outgoing $[(\rho\bar{q})_\beta \bullet \Delta\bar{A}]_n \ge 0$ $\quad \xi'_{l,n} = 1$
- Normalize: $\quad \xi_{l,n} = \xi'_{l,n} / \sum_{l=1}^{N}\xi'_{l,n}$
- Build: $\quad (\dot{\rho}V)_{\beta,m} = (\dot{\rho}V)_{\beta,m} - \sum_{n=1}^{N}\left\{\sum_{l=1}^{N}\xi_{l,n}[(\rho\bar{q})_\beta \bullet \Delta\bar{A}]_n\right\}_{m(l)}$

Momentum and energy equations, while having different accumulations, use the same distribution parameters.

The distribution satisfies the Lagrangian nature of the particle flow in a vacuum, absolute conservation and introduces only limited lateral diffusion.

CFD Computing Environment (Runtime Choices)



Code Development Strategy Supports Multi-CPU Parallel Processing

Keys to Success

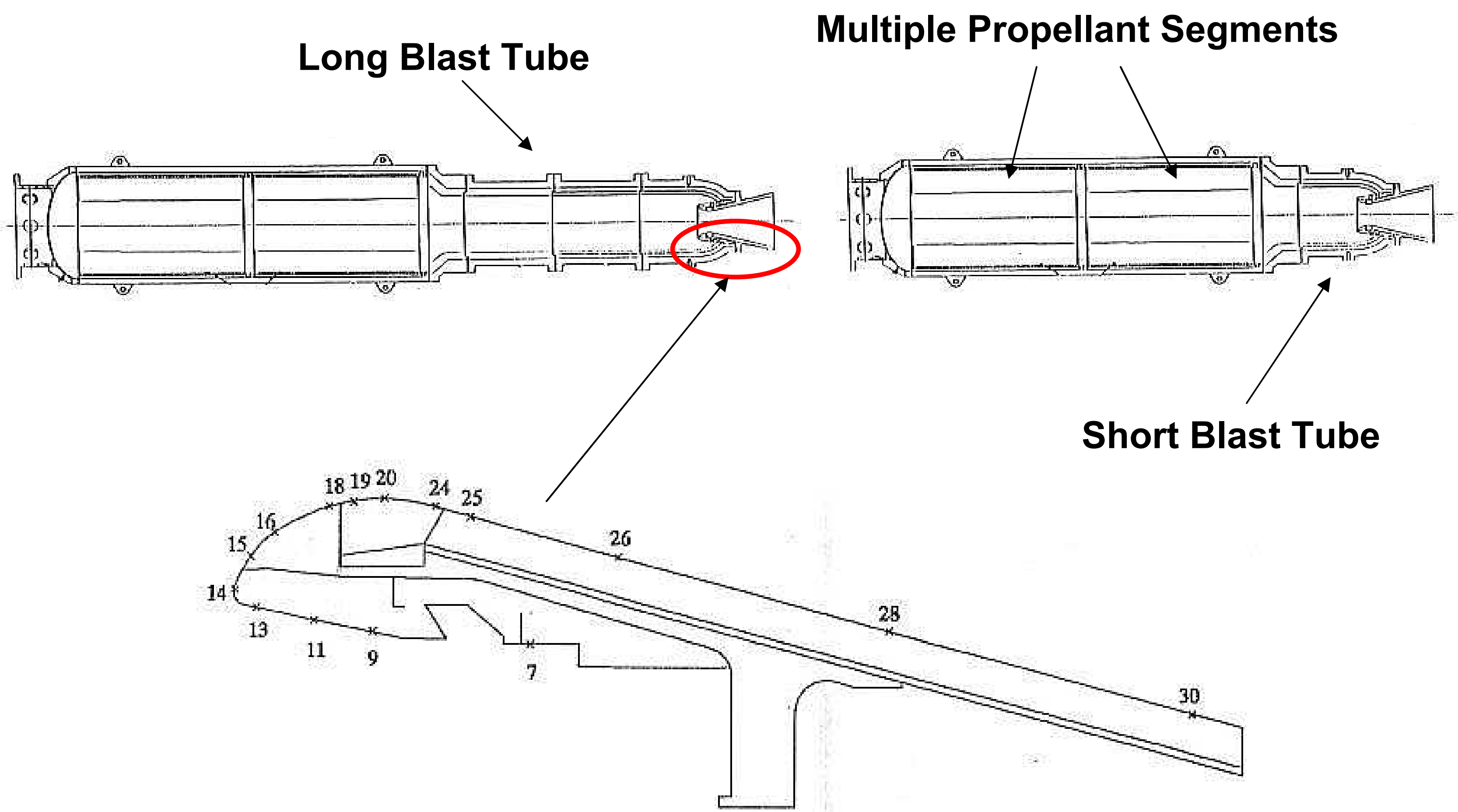
- Provide the features/physics outlined above - this is the starting point
- Validate the analysis by classical and experimental comparisons
- Demonstrate the applicability to off-design/unusual configurations
- Perform "closed envelope" solutions to selected problems of interest
- Demonstrate the ability to, for a given physics selection, successively refine the grid to determine grid density sensitivity
- Ascertain, for a given problem and a given grid, the sensitivity of the solution to physics models selection

MNASA Solid Rocket Motor Database Available for Model Validation

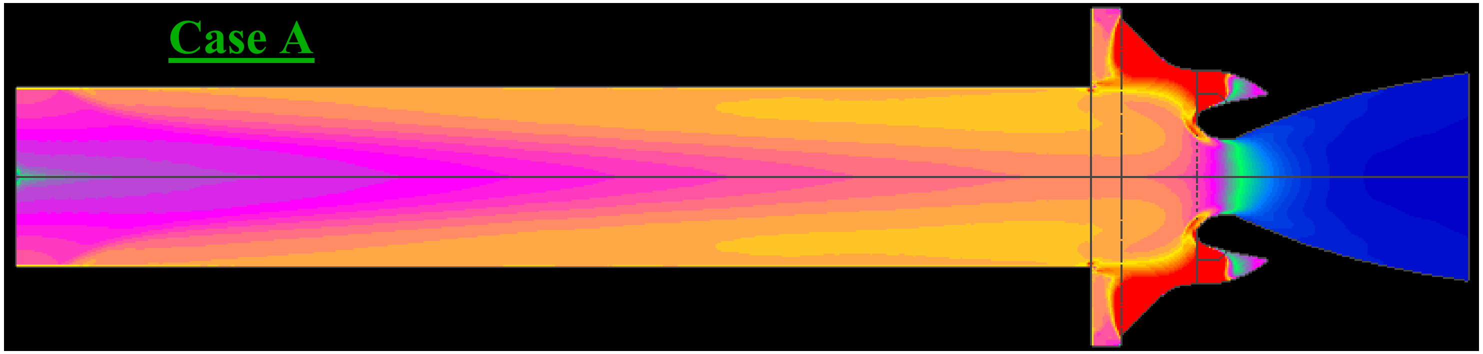
- MNASA motors firings were conducted at MSFC to study nozzle and insulation material response to motor environments
  - 48 Inch diameter motor, ~10,000 lbm propellant, 30+ second burn time
  - Tested with aluminized propellant, conventional nozzle materials
- Extensive database available from MNASA motors for model validation
  - Nozzle erosion measurements by station
  - Thermocouples at multiple locations
  - Pressure-time histories recorded
  - Plume particle data captured
- Analysis of MNASA motors leverages previous modeling experience
  - A number of two phase flowfield analyses have been conducted with various assumptions for particle size and distribution
  - Nozzle material response models have been developed and anchored with measured nozzle ablation data for a number of propellants, nozzle configurations, and ablative materials

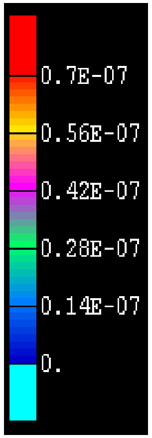
MNASA Motor Description

- **MNASA Motor data readily available**
  - **with multiple configurations**



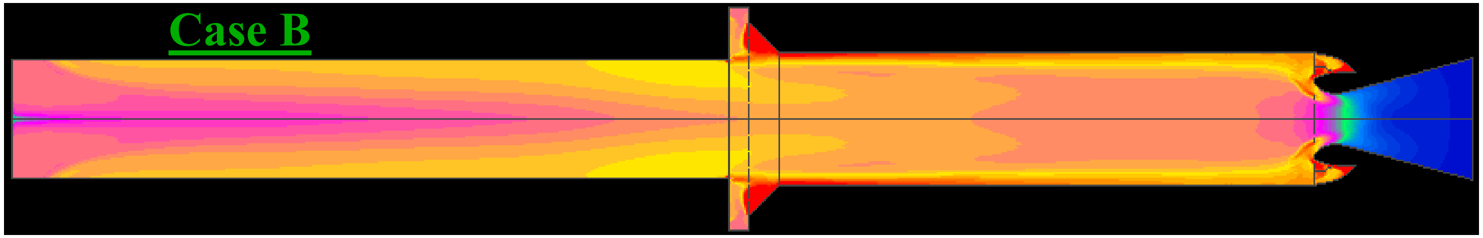
MaxS 2-Phase Flow CFD Analysis of 48-inch MNASA Motor: 2-microns Particle Density





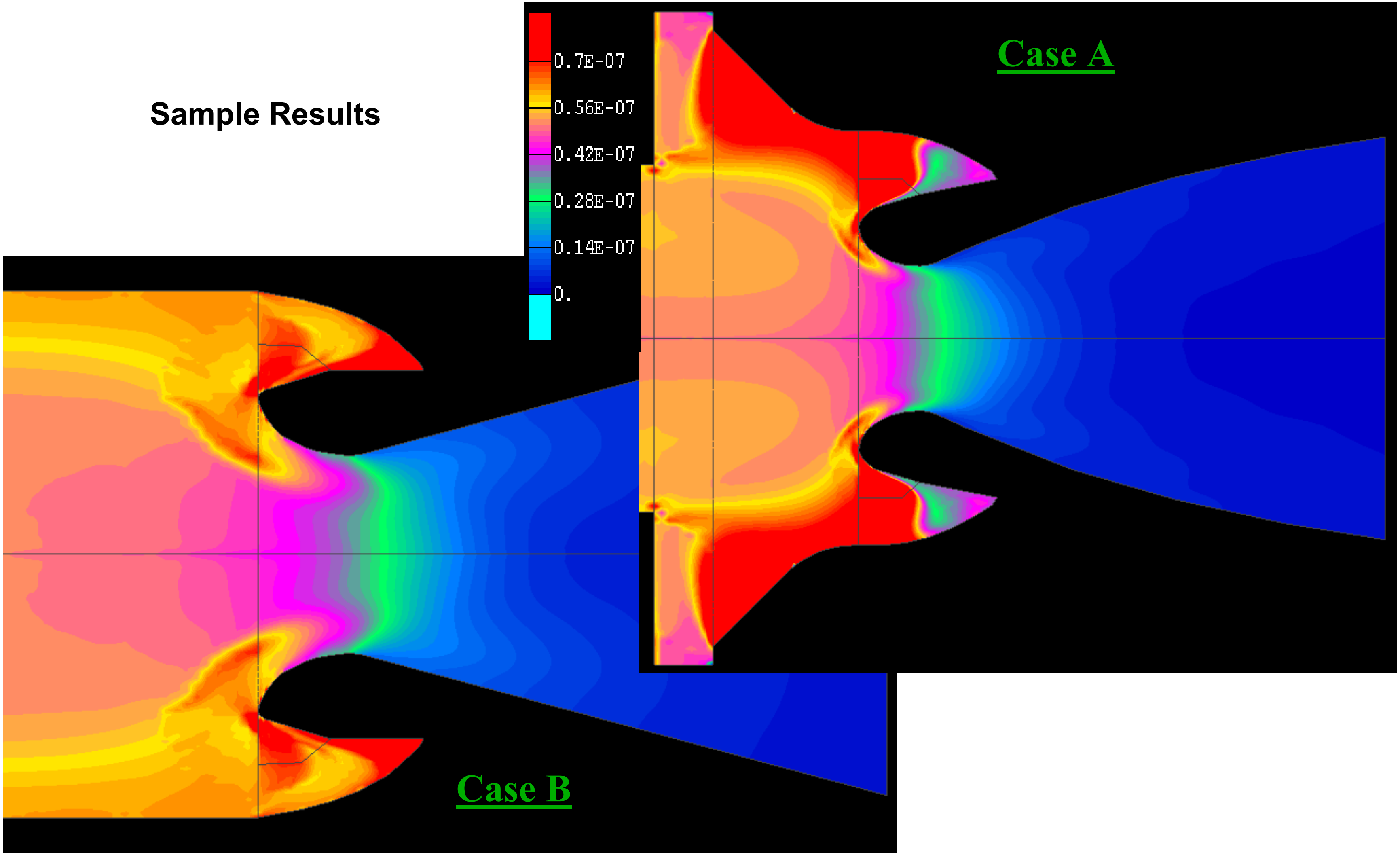
Case A : Configuration 1 (no blast tube, contoured nozzle)
- 2 micron diameter particulate

Case B : Configuration 2 (blast tube, conic nozzle)
- 2 micron diameter particulate



MNASA 48-inch Motors, Close Up of Nozzle: 2-microns Particle Density

Sample Results



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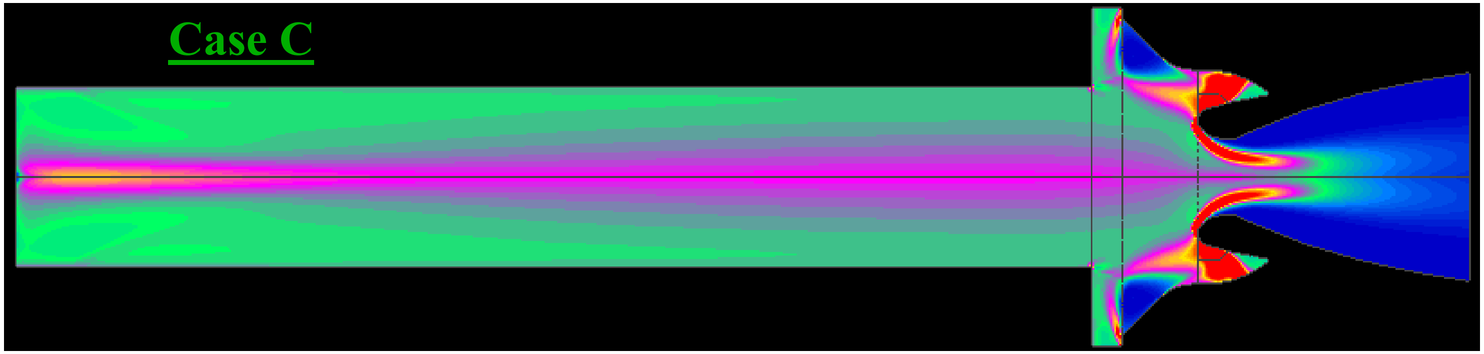
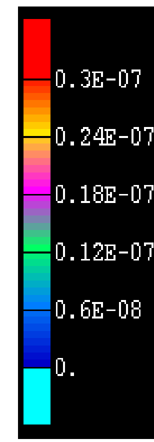
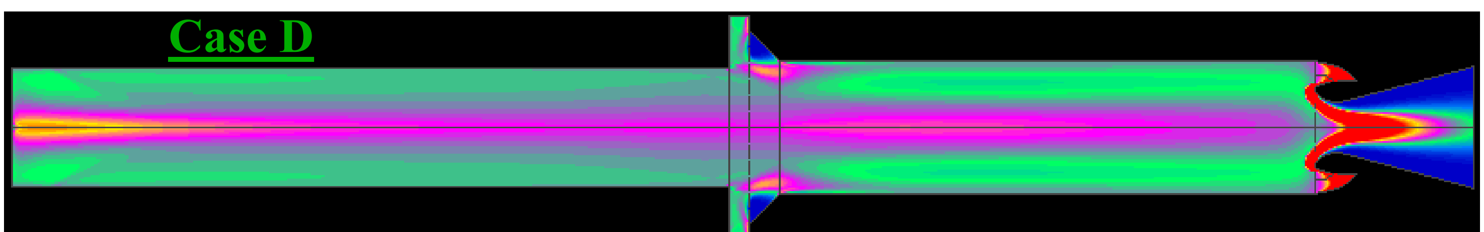
MaxS 2-Phase Flow CFD Analysis of 48-inch MNASA Motor: 80-microns Particle Density





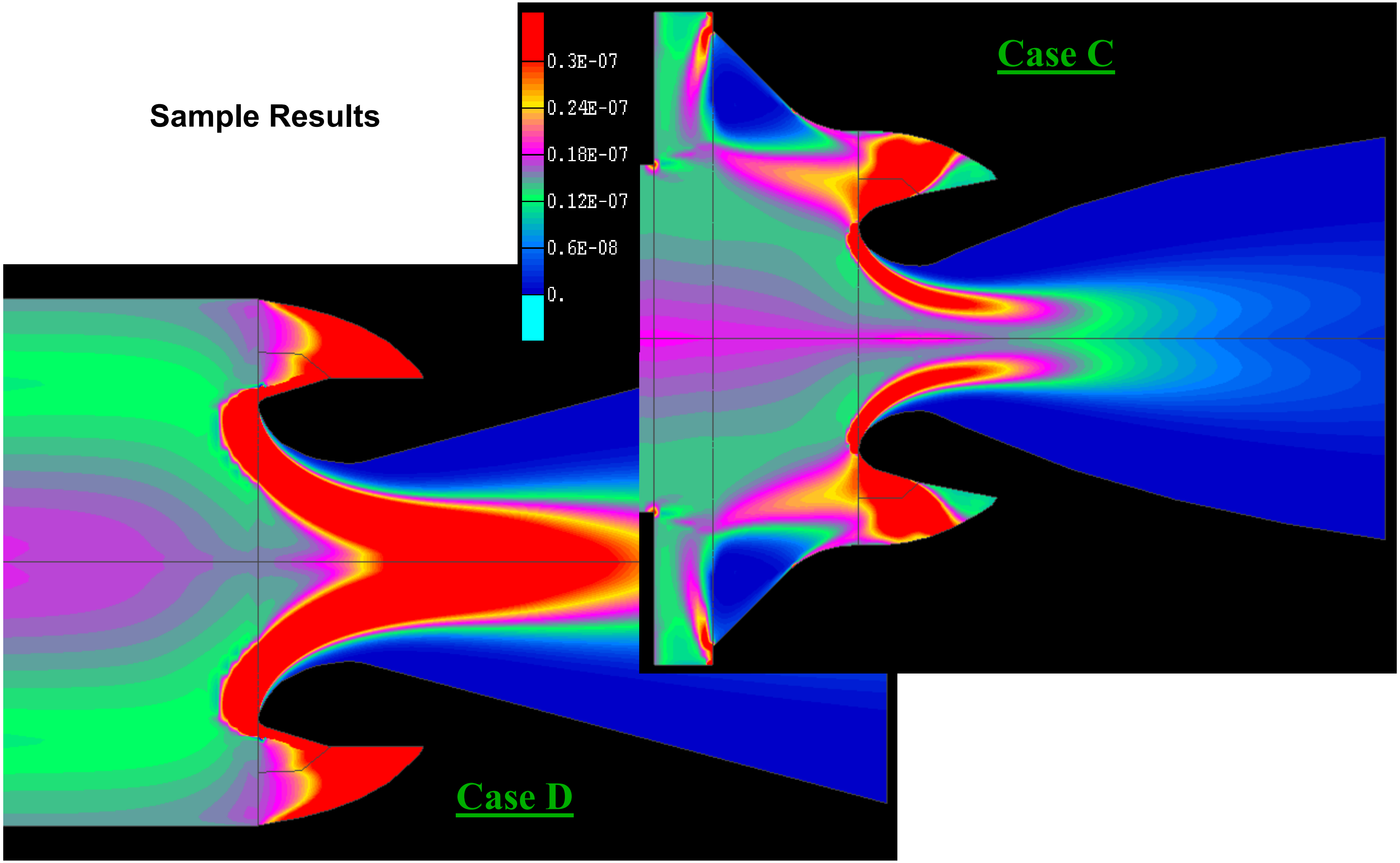
Case C : Configuration 1 (no blast tube, contoured nozzle)
- 80 micron diameter particulate

Case D : Configuration 2 (blast tube, conic nozzle)
- 80 micron diameter particulate



MNASA 48-inch Motors, Close Up of Nozzle: 80-microns Particle Density

Sample Results



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Concluding Remarks

- Prior MNASA SRM 2-phase flow CFD simulations analyzed using constant-sized particles
  - Existing G-law empirical model limited to this simplification
- New 2-phase flow model under development in this IHPRPT M&S effort will provide more realistic particle evolution model
  - Variable-sized particles will be available for material response models
- Validation plan for new model:
  - Model verification with closed-form solutions for simplified problems
  - Initial validation with existing cold flow and small SRM's
  - MNASA database and other existing large SRM's
  - Prediction for new SRM(s) to be tested as part of IHPRPT program